Comparison between a thermal and a time-dependent mean-field description of a two level bosonic model

M. C. Cambiaggio

Departamento de Fı´sica, Centro Ato´mico Constituyentes, Comisio´n Nacional de Energı´a Ato´mica, Avenida del Libertador 8250, 1429 Buenos Aires, Argentina

G. G. Dussel* and A. M. Szyferman

Departamento de Fı´sica ''Juan Jose Giambiagi,'' Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Pabello´n 1, Ciudad Universitaria, 1428 Buenos Aires, Argentina

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The thermal mean-field (Hartree-Bose-Bogoliubov) approximation is applied to a simple bosonic model that is related to the phase transition from spherical to deformed nuclei. Similarities and differences with the time-dependent approach are discussed, in particular, the sensitivity of each method for the detection of the phase transition. [S0556-2813(99)02710-7]

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I. INTRODUCTION

The Hartree-Bose-Bogoliubov (HBB) description of bosonic systems $[1,2]$ provides a single excitation image of the low energy part of the spectra of many body systems. The thermal $\lceil 3 \rceil$ and time dependent versions $\lceil 4 \rceil$ contain basically all the information related with the elementary excitations (of the single particle type) for the whole spectrum of the Hamiltonian considered. Nevertheless, the complexity of using each method as well as the information that they provide are different. In general, the thermal treatment can be used for any Hamiltonian while the time dependent version is very complicated to apply except for very simple Hamiltonians where one can isolate the relevant degrees of freedom. It is well known from the fermionic case $[5]$ that both types of treatments provide different descriptions of the excitations; the time dependent treatment is more complete while the thermal one isolates the excitations that have larger degeneracies.

In the present paper we apply the thermal treatment to a very simple bosonic model that has already been studied in its time dependent version. This simple two-level bosonic model has been used $\lceil 6 \rceil$ for studying the competition between a condensate of pairs of like particles and a condensate of α -like clusters. The former has been traditionally related to a superconductive description of nuclei as pairs of nucleons coupled to $J=0$, $T=1$, have been used in nuclear superfluidity $[7,8]$ as well as in pairing vibrations $[9]$. A condensate of α -like clusters, instead, may be associated with deformed states. $[10-13]$.

This simple two-level bosonic model $[6]$ presents a phase transition between a condensate of pairs of bosons and a condensate of bosons that strongly depends on the relations between the number of bosons and the degeneracies of the two levels. Details related with the selection of the appropriate parameters to scale this problem as well as the phase

transitions described using the time dependent treatment have been discussed in Ref. $[4]$

The purpose of the present paper is to apply a thermal mean-field approximation to the abovementioned bosonic model in order to study the phase transitions that occur in the system, not only for the ground state but also for higher excitation energies and compare the results obtained with the ones corresponding to the time dependent treatment. These excitation energies can be thought as related to the ''critical temperature'' at which the phase transition occurs.

In Sec. II we review the model studied and the results obtained in Ref. $[6]$. In Sec. III we review the timedependent mean-field approximation applied to the simple model and develop its thermal description. The results obtained are shown and discussed in Sec. IV.

II. THE MODEL AND ITS EXACT TREATMENT

The model consists of two nondegenerate shells of degeneracies 2 and 2*R* and single boson energies $-D/2$ and $D/2$. The two lower levels simulate the proton and neutron pairing ''bosons'' that are used in the usual description of pairing vibrations. A condensate of this type of bosons can be described as a superconductive system. The 2*R* upper levels simulate two-particle excitations formed by a proton and a neutron. If these proton-neutron excitations interact via a pairinglike residual Hamiltonian, one obtains collective pairs of proton-neutron pairs that may have the same quantum numbers as α particles. It has been shown [12] that this type of residual Hamiltonian has some resemblance with the effective interaction for the 212Po nucleus.

We will study the thermal description of a generalized version of this model, that was studied before using the timedependent version. In this extended model the level degeneracies are $2R_0$ and $2R_1$, respectively. The Hamiltonian is

*^H*⁵ *^D* ² F (*m*51 *R*1 ~^g *^m* † ^g *^m*1^g *m¯* † ^g *m¯* !² (*m*51 *R*0 ~b *^m* † ^b *^m*1^b *m¯* † ^b *m¯* !G ²*^G* (*m*,*m*8.0 g *m* † ^g *m¯* † ^b *m¯* ⁸ *On leave of absence from the Comisio ^b *^m*⁸ 1H.c., ~2.1! ´n Nacional de Energı´a

Atómica.

where $\gamma_m^{\dagger}(\beta_m^{\dagger})$ are boson creation operators in the level 1(0) and *G* is the interaction strength.

The exact solution may be found by diagonalization $[6]$. An important point when studying a simple model such as this is the selection of appropriate scaling parameters. In Ref. [6], where R_0 was equal to one, it has been shown that it is convenient to scale the energies with the parameter $GM\sqrt{MR_1}$ where *M* is half the number of bosons whereas the appropriate dimensionless interaction parameter is ξ $= D/(G\sqrt{MR_1})$. As the interaction has only off-diagonal matrix elements all the physical results are independent of the sign of *G*. It is also possible to change the sign of ξ by changing the sign of *D*. In what follows negative values of ξ will correspond to a change in the sign of *D*.

When the interaction is negligible the ground state of the system will be approximately described by a condensate of single bosons in the lower shell. As the interaction strength increases one expects a ground state phase transition to a condensate of a coherent combination of pairs of conjugate bosons. This phase transition has been found $[6]$ but only for negative values of the interaction parameter ξ , at $\xi=-1$, and in the limit $R_1 \rightarrow \infty, M \rightarrow \infty, M/R_1 \ll 1$. For positive values of ξ the ground state is always a condensate of pairs of bosons, no matter how large ξ (i.e., how small the interaction) may be.

The most striking result obtained in Ref. $\lceil 6 \rceil$ was that the number of α -like clusters was very high. Even for values of ξ as large as 2. one obtains a few percentage of α -like clustering in the approximate wave function. As the model Hamiltonian has similarities with the effective one obtained for the 208 Pb region [12], this may help to understand the high values of the preformation factor for α particles in this region $[14,15]$.

III. APPROXIMATE TREATMENTS

A. Time-dependent Hartree-Bose-Bogoliubov treatment

We will make a short review of the time-dependent variational approach following closely Ref. [4]. It is convenient to introduce the boson pair creation operators Γ_1^{\dagger} $=\sum_{m>0}^{R_1} \gamma_m^{\dagger} \gamma_m^{\dagger}$, $\Gamma_0^{\dagger} = \sum_{m>0}^{R_0} \beta_m^{\dagger} \beta_m^{\dagger}$ and the number operators $N_1 = \sum_{m>0}^{R_1} \gamma_m^{\dagger} \gamma_m + \gamma_m^{\dagger} \gamma_m^{\dagger}$, $N_0 = \sum_{m>0}^{R_0} \beta_m^{\dagger} \beta_m + \beta_m^{\dagger} \beta_m^{\dagger}$. With these definitions the Hamiltonian (2.1) is written as

$$
H = \frac{D}{2}(N_1 - N_0) - G(\Gamma_1^{\dagger} \Gamma_0 + \Gamma_0^{\dagger} \Gamma_1)
$$
 (3.1)

and the total number of bosons is $N=N_0+N_1=2M$.

To obtain the time-dependent (TD) Hartree-Bose-Bogoliubov equations, one has to use the time-dependent variational principle appropriate for non-normalized states $[16]$ with an action defined as

$$
S = \int dt \left[\frac{1}{2} i \frac{\langle \psi | \dot{\psi} \rangle - \langle \dot{\psi} | \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \right]
$$
(3.2)

and use $|\psi\rangle = |Z_0 Z_1\rangle = e^{\overline{Z}_0 \Gamma_0^{\dagger} + \overline{Z}_1 \Gamma_1^{\dagger}} |0\rangle$.

Although all calculations could be performed in terms of the variables Z_i , \overline{Z}_i , it is more convenient to introduce new variables which are canonical $[17,18]$:

$$
\omega_i = \sqrt{\frac{R_i}{1 - Z_i \overline{Z}_i}} Z_i.
$$
\n(3.3)

The dynamical problem has two degrees of freedom, the complex variables ω_0 and ω_1 . Therefore, the existence of two constants of motion, the energy and the number of particles, makes the system integrable. The most adequate variables for the integration are

$$
m = \frac{\omega_0 \overline{\omega}_0 + \omega_1 \overline{\omega}_1}{M},
$$

\n
$$
\varphi = \frac{1}{2} (\varphi_0 + \varphi_1),
$$

\n
$$
n = \frac{\omega_1 \overline{\omega}_1 - \omega_0 \overline{\omega}_0}{M},
$$

\n
$$
\alpha = \frac{1}{2} (\varphi_1 - \varphi_0),
$$
\n(3.4)

where $\varphi_i = \arg(\omega_i)$. Noting that $\omega_i \overline{\omega}_i$ is the mean number of pairs in level *i* one gets that *m* is conserved, $m=1$, and that the range of *n* is $-1 \le n \le 1$. The mean value of the Hamiltonian becomes

$$
\mathcal{H} = DMn - GM\sqrt{R_1 + \frac{M}{2}(m+n)}
$$

$$
\times \sqrt{R_0 + \frac{M}{2}(m-n)\sqrt{m^2 - n^2}\cos(2\alpha)}.
$$
 (3.5)

The TDHBB results are obtained solving the dynamical equations and the trajectories are best represented implicitly in the phase plane (n, α) as constant energy curves H $=$ const. It is clear that the appropriate scaling to be used depends on the relation between the number of pairs of bosons *M* and the degeneracies R_0 and R_1 . We have considered three different regimes in which it is convenient to scale the energies and interaction parameters in different ways.

(a) When $R_0 = 1$; $M < R_1$, it is convenient to scale the energies with the parameter $GM\sqrt{MR_1}$ and consider as the corresponding interaction parameter, $\xi = D/(G\sqrt{MR_1})$. The energy function (3.5) becomes $(fixing m=1)$

$$
\mathcal{E} = \frac{\mathcal{H}}{GM\sqrt{MR_1}}
$$

= $\xi n - \sqrt{1 + \frac{M}{2R_1}(1+n)}\sqrt{\frac{1}{M} + \frac{1}{2}(1-n)}\sqrt{1-n^2}$
× cos(2 α). (3.6)

(b) When $R_0 = R_1 = R$ (symmetric model) and $M \le R$. The appropriate energy scaling is *GMR* with an interaction parameter defined as $\varepsilon = D/GR$. Equation (3.5) becomes

$$
\mathcal{E} = \frac{\mathcal{H}}{GMR} = \varepsilon n - \sqrt{\left(1 + \frac{M}{2R}\right)^2 - \left(\frac{Mn}{2R}\right)^2} \sqrt{1 - n^2} \cos(2\alpha). \tag{3.7}
$$

(c) *M* greater than the degeneracies R_0 and R_1 . In the limit $M \ge R_0, M \ge R_1$, the appropriate energy scaling is GM^2 with an interaction parameter $\zeta = D/GM$ and an energy function

$$
\mathcal{E} = \frac{\mathcal{H}}{GM^2}
$$

= $\zeta n - \sqrt{\frac{R_0}{M} + \frac{1-n}{2}} \sqrt{\frac{R_1}{M} + \frac{1+n}{2}} \sqrt{1 - n^2}$
× cos(2 α). (3.8)

Comparing the exact ground state results obtained by diagonalizing the Hamiltonian (2.1) with the TDHBB energies it was concluded $[4]$ that the latter tend to the exact energies for large number of bosons and large degeneracies. Analyzing the minimum value of the scaled energy $\mathcal E$ as a function of the interaction parameter $(\xi, \varepsilon, \text{ or } \zeta)$ depending on the case considered) it was determined if there existed a phase transition from a condensate of single bosons in the lower level (normal state) to a condensate of a coherent combination of pairs of conjugate bosons (superconductive state).

In case (a) a ground state phase transition is found at ξ_c $= -\sqrt{1 + M/R_1}$ for $M \rightarrow \infty, R_1 \rightarrow \infty, M \leq R_1$. For positive values of the interaction parameter no ground state phase transition occurs. In the symmetric case (b) in which $R_0 = R_1$ $=$ *R* no ground state phase transition is found for *M* \leq *R*. On the other hand, when the number of bosons is greater than the degeneracies of the levels $\lceil \text{case (c)} \rceil$, analyzing Eq. (3.8) one finds two ground state phase transitions, one for positive values of the interaction parameter ζ and the other for negative values. The positive critical strength is $\zeta_c = \sqrt{1 + R_0 / M}$ and it is obtained in the limit $R_1 / M \rightarrow 0$ whereas for negative values one gets $\zeta_c = -\sqrt{1 + R_1/M}$ in the limit $R_0 / M \rightarrow 0$. Therefore, in the symmetric model, $R_0 = R_1 = R$, the ground state phase transition only occurs if $M \ge R$. Performing a similar analysis in the symmetric fermionic model (see Ref. $[17]$) the result obtained is quite different. In this case the ground state phase transition only occurs in the middle of the shell, i.e., for $M = R$.

B. The thermal treatment

We will now develop the thermal treatment for a boson system following closely the description done in Ref. $[19]$ for a fermion system. We start by considering a general twobody Hamiltonian

$$
H = \sum_{ij} T_{ij} b_i^{\dagger} b_j + \frac{1}{4} \sum_{ijkl} V_{ij,kl} b_i^{\dagger} b_j^{\dagger} b_l b_k, \qquad (3.9)
$$

which, as usual, is approximated by a one-body Hamiltonian describing noninteracting quasiparticles, i.e.,

$$
F = H - \mu N \approx \mathcal{H}_{\text{HBB}} = E_{00} + \sum_{i} E_{i} \alpha_{i}^{\dagger} \alpha_{i}, \qquad (3.10)
$$

where *F* is the free energy, the chemical potential μ is fixed by imposing the condition that the mean number of particles is well defined. E_{00} is the energy of the quasiparticle vacuum, E_i are the quasiparticles energies while α_i^{\dagger} creates one quasi-particle and is defined by the unitary transformation

$$
\alpha_i^{\dagger} = \sum_j \{ U_{ij} b_j^{\dagger} + V_{ij} b_j \}.
$$
 (3.11)

To obtain a thermal HBB description the density operator and the partition function that are defined as

$$
D = Z^{-1} e^{-\beta (H - \mu N)}, \tag{3.12}
$$

$$
Z = \text{Tr}\{e^{-\beta(H - \mu N)}\},\tag{3.13}
$$

on applying the HBB approximation, become

$$
Z_{\rm HBB} = \Pi_i \frac{1}{(1 - e^{-\beta E_i})},
$$
\n(3.14)

$$
D_{\rm HBB} = Z_{\rm HBB}^{-1} \Pi_i e^{-\beta E_i n_i}, \tag{3.15}
$$

where n_i is the quasiparticle number operator corresponding to the state *i* and

$$
f_i = \frac{1}{e^{\beta E_i} - 1}; \quad \beta = \frac{1}{KT}.
$$
 (3.16)

The usual density and pairing matrices are

$$
\rho_{ij} = \langle b_j^{\dagger} b_i \rangle = \text{Tr} \{ D b_j^{\dagger} b_i \} = [U^T f U^* + V^{\dagger} (1+f) V]_{ij},
$$
\n(3.17)
\n
$$
t_{ij} = \langle b_j b_i \rangle = \text{Tr} \{ D b_j b_i \} = -[U^T f V^* + V^{\dagger} (1+f) U]_{ij}.
$$
\n(3.18)

The energy is evaluated using Wick's theorem [2] for $T \neq 0$. One then obtains

$$
\mathcal{E}_{FT} = \text{Tr}\{D_{\text{HBB}}H\} = \text{Tr}\left\{ \left(T + \frac{1}{2}\Gamma\right)\rho + \frac{1}{2}\Delta t^{\dagger} \right\}, (3.19)
$$

where the HB Hamiltonian as well as the self-consistent and pairing potentials are defined as usual as

$$
\mathcal{H}_{\rm HB} = T - \mu + \Gamma, \tag{3.20}
$$

$$
\Gamma_{ij} = \sum_{k,m} V_{ik,jm} \rho_{mk},\qquad(3.21)
$$

$$
\Delta_{ij} = \frac{1}{2} \sum_{k,m} V_{ij,km} t_{km}.
$$
\n(3.22)

The coefficients *U* and *V* are obtained by solving the eigenvalue equations

FIG. 1. Critical temperatures as a function of the different strength parameters in the three different regimes: (a) $R_0 = 1$, R_1 = 500, and $M = 50$; (b) $R_0 = 50$, $R_1 = 50$, and $M = 50$; and (c) R_0 $=$ 50, R_1 = 50, and $M = 2000$.

$$
\begin{pmatrix} \mathcal{H}_{\text{HB}} & -\Delta \\ \Delta^* & -\mathcal{H}_{\text{HB}}^* \end{pmatrix} \begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix} . \tag{3.23}
$$

These equations are the FTHBB equations and, of course for $T=0$, they provide the usual HBB description.

FIG. 2. Results obtained for the $R_0=1$, $R_1=500$, and $M=50$ case. (a) The order parameter Δ_0 ; (b) the order parameter Δ_1 ; and (c) the ground state energy. All the magnitudes are multiplied by ξ .

We will now consider the equations obtained for the BCS limit, i.e., when the Hamiltonian can be written as

$$
H = \sum_{i} \varepsilon_{i} b_{i}^{\dagger} b_{i} - \sum_{i,j>0} G_{ij} b_{i}^{\dagger} b_{i}^{\dagger} b_{j} b_{j}, \qquad (3.24)
$$

FIG. 3. Results obtained with $R_0 = 1$, $R_1 = 500$, and $M = 50$ for $T = 0.4$. (a) the order parameter Δ_0 ; (b) the order parameter Δ_1 ; (c) the chemical potential μ ; (d) the ground state energy; (e) the free energy; (f) the quasiparticle energy E_0 ; and (g) the quasiparticle energy E_1 . All the magnitudes are multiplied by ξ to be properly scaled.

FIG. 4. Results obtained with $R_0 = R_1 = 50$ and $M = 50$. (a) The order parameter Δ_0 ; (b) the order parameter Δ_1 ; (c) the ground state energy; and (d) the specific heat. All the magnitudes are multiplied by ε .

where \bar{i} is related to *i* by the time reversal operation and ε_i includes the HB and chemical potentials.

In this case the FTHBB equations have a trivial structure. They are equivalent to gap and number equations that can be written as

$$
N = \sum_{i} \left[\frac{\varepsilon_{i}}{2E_{i}} \cot g h \left(\frac{\beta E_{i}}{2} \right) - \frac{1}{2} \right],
$$
 (3.25)

$$
\Delta_i = \frac{1}{2} \sum_{j>0} G_{ij} \frac{\Delta_j}{E_j} \cot g h \left(\frac{\beta E_j}{2} \right), \tag{3.26}
$$

where $E_i = \sqrt{\varepsilon_i^2 - \Delta_i^2}$ are the quasiparticle energies. The U_i and V_i satisfy now the normalization condition $U_i^2 - V_i^2 = 1$ and can be defined in terms of ε_i and Δ_i as $U_i^2 = \frac{1}{2}$
+ $\varepsilon_i/2E_i$, $V_i^2 = -\frac{1}{2} + \varepsilon_i/2E_i$.

In the simple model that we are considering, that has a constant pairing interaction acting only on two levels with energies $\mp D/2$ and degeneracies R_0 and R_1 , respectively, we must determine, for a given number of particles *N*, the unknowns Δ_0 and Δ_1 , as well as the chemical potential μ . With them we can evaluate the total energy of the system \mathcal{E}_{FT} and the specific heat, obtained through the numerical derivative of \mathcal{E}_{FT} with respect to *T*. In order to display the results it will be convenient to scale the gap parameters properly, depending on the values of R_0 , R_1 , and M .

IV. RESULTS AND DISCUSSION

In this work we have two main points of interest, one is the study of the temperature dependence of the different order parameters describing the system, the other one is the comparison between the description provided by the time dependent version and the one provided by the present treatment. It is well known that both approaches provide a complete description of the system under consideration but each one emphasizes different aspects and can explain in simple terms some of the properties of the system but have problems to describe, in a simple way, another ones. For example, in the previous work $[4]$ it was found in a very natural way a boundary between the different types of behavior of the system: it was possible to obtain the energies at which for a given strength the system changed from normal to a condensate of pairs of bosons. On the other hand it was quite complicated to obtain the value of the order parameter as

FIG. 5. Results obtained with $R_0 = R_1 = 50$ and $M = 2000$. (a) The order parameter Δ_0 ; (b) the ground state energy; (c) the free energy; and (d) the quasiparticle energy E_1 . All the magnitudes are multiplied by ζ .

function of the interaction strength.

To analyze the temperature dependent description we will use the experience obtained from the time dependent version, such as the fact that it is convenient to analyze the results obtained in each one of the three different regions discussed in the previous section. To find the boundary between the region where the system can be described as a normal one and that where it behaves as a condensate of pairs of bosons we solved the number $[Eq. (3.25)]$ and gap $[Eq. (3.26)]$ equations when the gaps just vanish. For a given interaction strength, the lowest temperature at which the gaps vanish can be defined as the critical temperature. In Fig. 1 we display these critical temperatures as functions of the corresponding strength parameters for the three different regimes. When trying to solve the gap and number equations as function of the temperature we found that they are not as well behaved as in the fermionic case $[5]$, i.e., they turn out to be unstable unless the initial guess for the parameters is close to the solution of the equations. This fact is due to the particular dependence of the quasiparticle energies on the gap parameter (the minus sign), that makes the quasiparticle energies small when the gap is different from zero but small.

We have also analyzed the behavior of the order parameters and other thermodynamical functions in each of the three abovementioned regimes.

(a) We consider the case $R_0 = 1$, $R_1 = 500$, and $M = 50$. In Fig. 2 we show the order parameters Δ_0 and Δ_1 as well as the ground state energy multiplied by ξ , in order to scale them properly as discussed in Sec. III A. For studying in detail the features of the phase transition we display in Fig. 3 the different order parameters and thermodynamical functions obtained at a fixed temperature. We choose $T=0.4$ because at this temperature the phase transition is clearly seen. We show not only the order parameters Δ_0 and Δ_1 but also all the relevant thermodynamical quantities properly scaled: the chemical potential, the ground state energy, the free energy, and the quasiparticle energies E_0 and E_1 . It is noticeable that it was possible to find metastable solutions. The different solutions were obtained following the different branches. For doing so we increased or decreased the strength parameter by a small amount and use as initial guess for the parameters the results obtained with the old strenght parameter, being able in this way to follow the branch into the metastable region, even if it has not the smallest energy. This is clearly seen by comparing Fig. $3(a)$ or $3(b)$ with Fig. $3(d).$

(b) We consider the case $R_0 = R_1 = 50$ and $M = 50$. In Fig. 4 we show the order parameters Δ_0 and Δ_1 , the ground state energy as well as the specific heat multiplied by ε . It is noticeable that the order parameters approach zero in a much milder way while the ground state energy has a richer structure than in the previous case. The specific heat shows a broad peak that corresponds to the phase transition as can be seen by comparing Fig. $4(d)$ with Fig. 1 (b) .

(c) We consider the case $R_0 = R_1 = 50$ and $M = 2000$. In Fig. 5 we show the order parameter Δ_0 [it must be noted that due to the symmetry of the model $\Delta_1(\zeta) = \Delta_0(-\zeta)$ making unnecessary to display it \vert ; the ground state energy, the free energy and the quasiparticle energy E_1 , multiplied by ζ .

Comparing the results obtained in the present work with the previous TDHBB ones we conclude that in the thermal treatment it is easier to evaluate the matrix elements of the two-particle transfer operators, related with the order parameters, than in the TDHBB treatment but on the other hand the obtention of the boundaries between the different types of behavior is much more complicated. In the TDHBB approach these boundaries are obtained in a simple way as analytical functions of the strength parameter while in the thermal treatment the gap and number equation are difficult to handle when the order parameters are close to zero because the convergence is not good.

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